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Quasiparticle Excitations in Valence-Fluctuation Materials: Effects of Band Structure and Crystal Fields*

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Abstract

Evidence is now quite strong that the elementary hybridization model is the correct way to understand the lattice-coherent Fermi liquid regime at very low temperatures. Many-body theory leads to significant renormalizations of the input parameters, and many of the band-theoretic channels for hybridization are suppressed by the combined effects of Hund's-rule coupling, crystal-field splitting, and the f-f Coulomb repulsion U. Some exploratory calculations based on this picture are described, and some inferences are drawn about the band structures of several heavy-fermion materials. These inferences can and should be tested by suitably modified band-theoretic calculations. We find evidence for a significant Baber-scattering contribution in the very-low-temperature resistivity. A new mechanism is proposed for crossover from the coherent Fermi-liquid regime to the incoherent dense-Kondo regime.

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I. Introduction

It is well known that single-impurity models, or more correctly, models with active sites behaving incoherently, are generally adequate to explain the behaviors of valence-fluctuation (VF) materials at high temperatures [1,2]. In fact, this type of model works surprisingly well down to rather low temperatures, $T \sim T_K$. At still lower temperatures, however, effects due to coherence between the active sites become dominant. Prominent examples of coherence effects are the insulating gaps (or pseudogaps) for certain "ionic" compounds (SmB_6, YbB_{12}, gold SmS, and TmSe), and a sharp Fermi surface for $CeSn_3$ (and thus, presumably, for all other intermetallic VF compounds). These effects indicate that at sufficiently low temperatures the "normal" VF materials behave as periodic Fermi liquids, in the manner described so elegantly by Luttinger [3]. This important conclusion was drawn especially by Martin and Allen [4]. Other effects attributed to coherence within intermetallic VF compounds are a strong decrease in resistivity [5], and a peak in "γ" (specific heat/temperature) [6].

Important goals at this time are thus to understand (a) the nature of the low-temperature coherence, and (b) the apparent breakup of this coherence with increasing temperature. We shall argue in some detail that the hybridization model holds the key to (a), and we shall then draw some inferences from this, based on simple model calculations. Although we shall be focusing on some common (but not universal) features, we want to emphasize that the very-low-temperature properties of real materials exhibit a significant degree of diversity, i.e., they have individual characteristics which cannot be adequately described simply by an appropriate choice of a characteristic "fluctuation" or

"Kondo" scaling temperature. We suggest a simple modification of conventional band theory, which should enable one to calculate the necessary ingredients for more realistic modeling of these individual features. We also outline a mechanism which we believe is responsible for breakup of the very-low-temperature coherence.

II. Renormalized Hybridization Model

The hybridization model, involving elementary hybridization between an ordinary conduction band and a zero-bandwidth lattice of localized orbitals, is probably the simplest model for describing a periodic VF system. Its relevance for VF materials was apparently first proposed by Mott [7] on intuitive grounds, although there were clear precedents by Coqblin and Blandin [8], and Doniach [5]. This type of model has since been obtained as the result of several approximate treatments of Anderson-lattice or Kondo-lattice Hamiltonians: Hartree-Fock approximation [9], Hubbard I approximation for Green's functions [10], and static approximation within the functional integral method [11]. It is well known that this model has considerable empirical validity for the ionic compounds with small insulating (semiconducting) gaps [4,12,13]: SmB_6, YbB_{12}, SmS (with only a pseudogap), and TmSe. There is also some experimental evidence [14] suggesting a similar quasiparticle state density for intermetallic VF compounds, where the electron number necessarily keeps the Fermi level ε_F away from the hybridization gap.

The plausibility of such a simple description is greatly strengthened by the observation that a result at least somewhat like this is to be expected if the Luttinger picture is correct for these materials.

In simplest terms, this picture assumes that the system would evolve continuously if the two-body interaction (here the Hubbard U) were to be switched on adiabatically. There is no adequte theoretical criterion to determine whether this picture must hold for VF materials (or for any other material [3]). Nevertheless, the experimental evidence seems quite clear that this is valid here. There are previous examples where a Fermi-liquid picture holds in spite of very strong short-range repulsions, namely liquid ^{3}He and nuclear matter. The concept of continuity with respect to U implies that there must be considerable similarity between the U = 0 case, for which the hybridization model is obviously correct, and the true situation with large U.

We have recently presented a new justification [15] for the hybridization model, based on a variational treatment of the ground state for Anderson lattice Hamiltonians. Although this method presumes the validity of the Luttinger picture, without proving it, this work has provided considerably more detail to date than previous ab initio studies. In effect, we express the many-body electronic ground state as

$$\Psi = \Omega\Phi_o \quad , \tag{1}$$

where Φ_o is a single-determinant wavefunction representing an appropriate uncorrelated (U = 0) reference state. All correlations are symbolized here by the wave operator Ω. After optimizing the ground state with respect to the variational parameters (here concealed within Ω), we generate quasiparticle excitations by a direct implementation of the original Landau definition [16],

$$\varepsilon_{qp}(k\sigma) = \delta E_{total}/\delta n_{qp}(k\sigma) \quad . \tag{2}$$

We do this by identifying the quasiparticle occupation numbers $n_{qp}(k\sigma)$ with the "bare" occupation numbers for the reference state Φ_o. For example, to determine ε_{qp} for a state $k\sigma$ with $k > k_F$, we add an electron in state $k\sigma$ to Φ_0; $\varepsilon_{qp}(k\sigma)$ is the corresponding change in $\langle H \rangle$.

This approach has a number of appealing features [15]. (1) It leads to a direct and faithful realization of the Luttinger picture of a periodic Fermi liquid. The Luttinger sum rule is obviously satisfied, and therefore the Fermi surface can be reliably determined. There is also a discontinuity in the true conduction-orbital occupation numbers at ε_F. (2) This provides a simple explanation for the renormalization to a low (kondoesque) temperature scale. It also emphasizes that there is a continuum of behavior between the "valence fluctuation" or strongly-mixed-valence regime, with characteristic temperatures typically $\gtrsim 10^2$K, and the "Kondo lattice" regime, with near-integer valence and characteristic temperatures $\lesssim 10^2$K. The "heavy fermion" materials are viewed as extreme examples of the latter, with characteristic temperatures $\lesssim$ 10K. (3) The general results exhibit a number of close correspondences with previous results for the single-impurity Anderson model. For example, although the simplest version of our work (the "one parameter" version, with one variational parameter per Bloch state k) corresponds directly to the simple hybridization model, and has a Wilson ratio of unity, there is also a more elaborate "two parameter" version. The latter has a Wilson ratio $\neq 1$, and has an f-electron spectral density resembling the two-peak structures found theoretically for the Anderson model, and seen in photoemission data for a number of cerium compounds. The "second" photoemission peak appears at a considerable distance from ε_F, and should therefore not interfere with the structure

near ε_F which determines low-temperature behavior. (This remains to be verified, however.) Taken together, these features strengthen our confidence in the results.

In view of the above developments, both experimental and theoretical, it now seems clear that the hybridization model must be taken seriously. It is therefore appropriate to explore its consequences in more detail than has been done previously. That is the main point of this report. In the following, we describe some initial steps in this direction.

We focus mainly on the heavy-fermion systems, where the characteristic temperature scale is extremely low, and especially on the examples ($CeAl_3$, $CeCu_6$, and some $CeCu_2Si_2$ samples) which remain "normal" (neither superconducting nor magnetic) at the lowest temperatures. These materials can be particularly instructive because their low-temperature anomalies should be least obscured by crystal-field-excitation or phonon effects. In most cases (UBe_{13} appears to us to be an exception), the crystal-field ground state of the "magnetic" configuration is simply a Kramers doublet. (The familiar $1/N_f$-expansion arguments about high ionic degeneracy are thus not relevant here.) Our theoretical point of departure can therefore be the simplest type of Anderson lattice, with no orbital degeneracy.

In the simplest model of Ref. 15, the quasiparticle spectrum was found to have exactly the form of the elementary hybridization model, but with two types of renormalization: (a) the bare f-electron level is shifted, $\varepsilon_f \rightarrow \tilde{\varepsilon}_f = \varepsilon_f + \mu$, (b) the d-f hybridization matrix elements are all reduced by a common factor, $V_k \rightarrow \tilde{V}_k = V_k(1-\xi)^{1/2}$, where ξ is the fractional occupation of the magnetic configuration. For ξ near unity

(the Kondo regime), this leads to very small $\tilde{V}_k$'s, and consequently to a very low characteristic temperature. Similar renormalizations have been found by means of the functional-integral formalism [11].

The conduction and localized Bloch orbitals simply hybridize, for each k, and produce two quasiparticle states,

$$\mathcal{E}_k^{\pm} = \frac{1}{2}\{\varepsilon_k + \tilde{\varepsilon}_f \pm [(\varepsilon_k - \tilde{\varepsilon}_f)^2 + 4\tilde{V}_k^2]^{1/2}\} \quad . \tag{3}$$

For initial orientation it is reasonable to consider a constant conduction-band density of states, $\rho_o = 2/W$ (W = conduction bandwidth, the 2 for spin degeneracy), and a constant $\tilde{V}_k \to \tilde{V}$. The resulting quasiparticle state density is

$$\rho(E) = \frac{2}{W}\left[1 + \frac{\tilde{V}^2}{(E-\tilde{\varepsilon}_f)^2}\right] \quad . \tag{4}$$

Due to the band limits of ε_k, this $\rho(E)$ has a small but finite gap between two sharp spikes, the latter arising from the flattening of the quasiparticle bands near the gap edges. For intermetallic systems the Fermi level ε_F should fall <u>within</u> one of these sharp peaks, and fairly close to the nearest gap edge.

III. Specific Heat

In Ref. 15 we noted that the curvature of this $\rho(E)$ is positive, and therefore the "linear specific heat coefficient" $\gamma \equiv C/T$ should initially increase quadratically as T rises from zero. This γ should then pass through a maximum and decrease, when the Fermi function broadens sufficiently to sense the gap, then at higher T it should exhibit a <u>second</u> maximum (or perhaps only a shoulder) when the Fermi

function broadens enough to include the other peak, on the far side of the gap. We consider it quite significant that all three of the "normal" heavy-fermion materials ($CeAl_3$, $CeCu_6$, and some $CeCu_2Si_2$) do indeed exhibit two structures of this type [6,17,18]. All three show quite distinct first peaks in C/T, well below 1K. Their second (higher-temperature) structures are mild peaks in C, with peak positions between 2K and 4K. (These second structures are only faint shoulders in plots of C/T.) UBe_{13} shows a very similar "second" structure [18], but no "first" peak, presumably because the latter is cut off by the superconducting transition.

We have now carried out a series of model calculations, in an attempt to qualitatively reproduce this behavior. For the above constant-ρ_o, constant-$\tilde{V}_k$ model there were two significant results. The temperature of the first peak is <u>very</u> low, only around 10% of $|\varepsilon_F - E_{nge}|/k_B$, where E_{nge} is the position of the near gap edge. (Compare with the Schottky anomaly ratio of 0.41.) This seems consistent with the data (see discussion in Ref. 15), and is therefore encouraging. On the other hand, the height of the γ peak was very small, exceeding the T = 0 value by only a few percent of this value, in contrast to the several 10's of percent seen experimentally.

We have tried to remove this discrepancy by adding more realistic features to the model. We substituted a semi-elliptic conduction state density, $\rho_o(\varepsilon_k) = (8/\pi W)[1 - (2\varepsilon_k/W)^2]^{1/2}$. This rounded off the tips of the sharp spikes in $\rho(E)$, but also pushed ε_F a bit farther from the gap edge, leaving the specific heat almost unchanged. We also considered the temperature dependence of the parameters ξ and μ, which make the quasiparticle energies (3) temperature dependent. The temperature

dependence of the chemical potential ζ (which plays a major role in the specific heat calculation) was changed by just the same amount as that of the $\mathcal{E}_k$'s near ε_F, leaving the important <u>differences</u> $\mathcal{E}_k - \zeta$ within the Fermi function essentially unchanged. (This must obviously be so, to conserve electrons.) The resulting change in specific heat was insignificant. We then turned to the k-dependnece of $\tilde{V}_k$, considering various plausible assumptions. Since d and f orbitals have opposite parity, we first tried $\tilde{V}_k \sim \sin(\pi k/k_{max})$, as compared to $\varepsilon_k \sim \cos(\pi k/k_{max})$, whereby $\tilde{V}_k \sim [1 - (2\varepsilon_k/W)^2]^{1/2}$. This allowed the gap to collapse. There were still two rounded peaks in $\rho(E)$, but this ρ now vanished only at the point $E = \tilde{\varepsilon}_f$, leaving only a pseudogap. The "first peak" in C/T disappeared completely.

We have found only one type of model able to explain the large magnitudes of the observed first peaks, and yet be plausibly consistent with the requirements of band theory. This is based on the explanation for the insulating gap of SmB_6 [4,12]. This model has a simple band dispersion, $\varepsilon_k \sim \cos(\pi k/k_{max})$, but $\tilde{V}_k \sim \sin(\pi k/2k_{max})$ is less obvious. Of course the latter vanishes at k = 0 (the Γ point), due to the opposite parity of d and f orbitals, but it is <u>maximum</u> at the zone boundary. The monotonic increase of $|\tilde{V}_k|$ all the way to the zone boundary causes one of the qp bands ($\mathcal{E}^+$ or $\mathcal{E}^-$, depending on the sign of the ε_k dispersion) to become <u>extremely flat</u> near the zone boundary, and thus to produce an extremely sharp spike in $\rho(E)$. For a given k_F, the contrast between the $\rho(E)$ maximum near the zone boundary, and $\rho(\varepsilon_F)$, can thus be much larger than for the case of constant $\tilde{V}_k$. This leads to a more prominent first peak. Even with this mechanism, however, to obtain a magnitude comparable to observation (17% rise beyond γ at T = 0 for $CeCu_6$, 60% for $CeAl_3$, 90% for $CeCu_2Si_2$) we found it necessary to have k_F

rather small, not more than 1/4 of the zone-boundary value k_{max}. At first sight, it might seem implausible that this would occur in all of these "normal" heavy-fermion materials. On the other hand, the extremely large T = 0 values of γ require "unusually" small values of $|\tilde{V}_k|^2$ at the Fermi surface. Such a common correlation between small k_F and heavy-fermion behavior therefore does have some plausibility.

The reason for $\tilde{V}_k$ having a slower k-dependence than ϵ_k is interesting, although at first sight it is quite specific for the SmB_6 structure. Within each octahedral B_6 cluster, the p orbitals combine to make effective d-like orbitals, and the centroid energies of the latter are rather close to those of the 5d orbitals of the Sm ions [19]. The d bands of this CsCl-like structure are therefore quite similar to the d bands for a BCC lattice, except that there is a splitting (with gaps) at the true SC zone boundary, because the two types of d orbitals are not perfectly equivalent. The main contribution to $\tilde{V}_k$ comes from overlaps between the Sm 4f's and the effective d's on the neighboring B_6 clusters. Noting that the B_6-Sm separation (as measured along one of the cubic axes) is only half of the Sm-Sm separation, it becomes clear why the k-dependence of $\tilde{V}_k$ is only half as rapid as that of the apparent d-band dispersion. We now speculate that something like this may be rather common. All of the "heavy fermion" and "Kondo lattice" materials are intermetallics containing ligand (non-RE) ions closer to the rare-earth (or actinide) ions than the smallest RE-RE separation. These ligands may well have a similar effect on $\tilde{V}_k$ even if their most important orbitals do not have effective d symmetry. (For p-like orbitals the present picture may be inverted: $\tilde{V}_k$ maximum at Γ and vanishing at k_{max}, with k_F near k_{max}.) This issue can and should be explored via band-theoretic calculations, as explained below.

Although this model appears to be adequate for the first peaks, we find that it fails to explain the second peak. To explain both peaks simultaneously, it appears necessary to assume a conduction-band structure with more than one branch intersecting $\tilde{\varepsilon}_f$ and the nearby Fermi level ε_F. This is, of course, very likely to be true for the complicated materials we are dealing with. With more branches, and with V_k's of different strengths (and possibly different k-dependences) for the various branches, there are obviously more possibilities. (Regardless of the number of branches, all of the different V_k's become renormalized by the same factor $(1-\xi)^{1/2}$.) We have not yet done any model calculations for this case.

IV. Transport Properties and the Kondo Crossover

In Ref. 15 we argued that the low-temperature conductivity should be calculable by a fairly conventional formulation,

$$\sigma(T) = \int \sigma(e) \left(-\frac{\partial f}{\partial E}\right) dE \quad , \tag{5}$$

where

$$\sigma(E) = \frac{e^2}{3} \lambda(E)\, v_{gr}(E)\, \rho_c(E) \quad . \tag{6}$$

This formulation assumes translationally-invariant quasiparticles, with the resistance due entirely to crystal imperfections; the interaction between quasiparticles is neglected. Here $\lambda(E)$ (the mean free path) and $\rho_c(E)$ (the conduction-electron state density) are slowly varying, and for an orientation may be considered constant, except for the gap in $\rho_c(E)$. The main variation within $\sigma(E)$ is thus due to the group velocity,

$$v_{gr} = \frac{1}{\hbar}\frac{\partial \mathcal{E}}{\partial k} = \frac{1}{\hbar}\frac{\partial \varepsilon_k}{\partial k}\frac{\partial \mathcal{E}}{\partial \varepsilon_k} = v^c_{gr}\frac{\partial \mathcal{E}}{\partial \varepsilon_k} \quad . \tag{7}$$

Observed resistivities typically show a quadratic behavior at extremely low T, $\rho = \sigma^{-1} = \alpha + \beta T^2$, with $\beta > 0$. This implies that $\sigma(E)$ should have negative curvature near ε_F. However, the derivative $\partial\mathcal{E}/\partial\varepsilon_k$ is easily seen to have positive curvature, over much of its range. Even assuming $\varepsilon_k \sim \cos(\pi k/k_{max})$, $\partial\varepsilon_k/\partial k \sim \sin(\pi k/k_{max}) \sim [1 - (2\varepsilon_k/W)^2]^{1/2}$, which has negative curvature, and also including a semi-elliptic conduction state density $\rho_o(\varepsilon_k)$, which has a similar effect, our $\sigma(E)$'s all retained a net positive curvature at ε_F.

It appears to us that the resolution of this impasse requires Baber scattering [20], as was already suggested for $CeAl_3$ a decade ago [21]. This process involves scattering between thermally-excited quasiparticles due to the effective quasiparticle interaction. This process also requires the existence of at least two quasiparticle bands, and these must have very different effective masses [20]. We have just argued, however, that two (or more) branches of the conduction-band manifold are indeed likely to intersect ε_F. Their combined hybridization with the f orbitals can easily be seen to lead to widely differing effective masses. Some of the "extra" qp bands would necessarily have small effective masses at ε_F, close to those of the bare conduction branches.

At somewhat higher but still very low temperatures, the Kondo-lattice and heavy fermion materials often show a very steep rise in resistivity, climbing to a peak many times greater than the T = 0 value, followed by a slight drop to a plateau which may have a slow (log T, Kondo-like) decrease [18]. It does not seem possible to explain this enormous rise by means of $\sigma(E)$ or Baber scattering, and for the heavy-

fermion cases the energy scale is clearly too small to be explained by crystal-field excitations. The Kondo-like behavior obviously cannot be explained either, by any of these mechanisms. We therefore turn to the ultimate limitation of the hybridization model -- a mechanism which we believe is responsible for the crossover between the low-T Fermi liquid behavior and the higher-T "dense Kondo" behavior.

The quasiparticle branch on the far side of the gap (side opposite from ε_F) is obtained [15], via (2), by altering the occupation numbers of the f orbitals (in Bloch representation) within the Φ_o of (1). Thanks to this "f character", the excitation of a qp state from this "far" branch alters each one of the system's N sites by an amount 1/N, which is equivalent to fully altering N/N = 1 site. In the simplest (one-parameter) version, the nature of this alteration is to prevent hybridization and leave the site in a pure magnetic (f^1-like or f^{13}-like) configuration. In the two-parameter version spin-flip scattering becomes possible for this site, which is the key feature for Kondo resistivity. Details have not been worked out, but we presume that this qp excitation effectively creates one site exhibiting incoherent Kondo-like resistive scattering. Excitation of a significant number of quasiparticles (a macroscopic fraction of N) from the "far" branch can thus cause a drastic change in the transport properties, and even in the quasiparticle spectrum itself [see Sec. 6H of Ref. 15]. Kondo behavior is thereby "turned on" in a continuous manner with increasing T. This crossover should lead to a Curie-law magnetic susceptibility at high T, as is also true for the hybridization model, but the Curie constant should differ from the prediction of the latter model. This crossover would not necessarily cause much change in the specific heat, however.

A related crossover was predicted long ago by Doniach [4], who called this "dehybridization". His mechanism proceeds by means of a rapidly-growing ($\sim T^2$) imaginary part for the self-energy (within the Green's function), which is thus a consequence of the Baber quasiparticle scattering. We agree that this mechanism should also be present, but this is different and considerably less radical than the present mechanism for Kondo crossover.

If the resistivity treatment (5)-(6) were really valid, the same $\sigma(E)$ would be appropriate for use in the standard expressions [22] for other transport properties. However, the presence of a spin-flip scattering component invalidates such a simple procedure. We could of course imagine using a temperature-dependent $\sigma(E)$, and this might well succeed in relating resistivity to thermopower. But even this would be unreliable for the magnetic properties (magnetoresistance and Hall effect), because of the well known fact that a magnetic field reduces spin-flip scattering. Nevertheless, the predictions of this simple approach, for gross features and correlations between the various properties, do seem to have considerable empirical validity [15].

V. Modified Band Theory

The preceding inferences about conduction-band structures and V_k's are obviously speculative, and need to be tested by suitable detailed calculations. We now suggest a method for doing this, via simple modifications of a conventional band-structure program. The basic idea is to simply "switch off" the V_k hybridization, in order to determine the form of the conduction bands in its absence. The f's should be treated as core orbitals, but with the degree of f filling set equal to the

average f occupation determined experimentally. This numerical calculation should be considerably easier than the conventional band problem. Symmetry analysis of the band branches in the vicinity of ε_F should also be easier. The final step will surely be considerably harder, however. That is to use tight-binding arguments to deduce the form of the various V_k's, considering only the conduction-f transitions allowed by Hund's-rule and crystal-field considerations, together with the large Hubbard U. One should thereby obtain reasonable imputs for the type of model calculations discussed here, recognizing of course that the magnitudes of the V_k's may be quite poorly determined.

This procedure takes account of the fact that much of the conduction-f hybridization incorporated in conventional band calculations is actually unphysical, being suppressed by the above ionic mechanisms, while the part that does survive is subject to renormalization, often very strong. The same ionic mechanisms should also greatly reduce the effect of direct f-f transfer, so that even for cerium it may be reasonable to neglect this process. On the other hand, cases where U is not very much larger than the ordinary band-theoretic width of the f's, as may be presumed for the paramagnon (T_3 log T specific heat) materials UAl_2 and UPt_3, may well require a more elaborate basic many-body theory.

There is of course much precedent for this procedure. Band calculations of this type have been done by a number of investigators, with various motivations. Most of these [23] have not been subsequently analyzed to obtain the relevant hybridizations. The many studies of "reference" materials, with empty or filled f shells, are clearly in the same spirit. There are also a few calculations [24] determining the hybridization elements, used as input for many-body theories of magnetic materials. A modified band calculation has just been completed for $CeAl_3$ [25], and is now being analyzed from the present standpoint.

IV. The Role of Crystal-Field Splitting

One effect of crystal-field splitting has already been mentioned: reduction of the magnetic-configuration degeneracy from (2J + 1) to that of the CF ground state, typically a Kramers doublet. This applies also to the $U^{3+} = 5f^3$ configuration in uranium compounds. The lack of a magnetic ground state in many uranium compounds strongly suggests that their $U^{4+} = 5f^2$ configuration has a singlet ground state, in agreement with the point-charge model [26]. Such uranium compounds should therefore have hybridization models very similar to those for Ce compounds. For example, this is very likely an important part of the reason why the resistivities of UBe_{13} and $CeCu_2Si_2$ look so similar [18]. We therefore believe that CF effects <u>are</u> present and are very important in uranium compounds; why more direct evidence for this is difficult to obtain is unclear.

Evidence for CF excitations is clear for a number of VF materials, for example $CeAl_3$, where there are two excited doublet levels [27]. These can be incorporated within the hybridization model by simply starting with several (in this case 3) different f levels, to be hybridized with the various conduction bands. The renormalization shift $\tilde{\varepsilon}_f - \varepsilon_f = \mu$ is identical for all of these levels, leaving their CF splitting unchanged.

If the CF excitation energies are large compared to representative values of $\Gamma = \pi|\tilde{V}_k|^2\rho_o(\varepsilon_k)$ for hybridization with these excited levels, the details of their hybridization structures (gaps vs. pseudogaps, etc.) become unimportant, and a more crude description such as Lorentzian resonances in $\rho(E)$ should be adequate for these excited levels. (Caveats about the Kondo crossover remain, however.) These

excited levels would then be treated essentially as in the model of Sales and Wohlleben [1]. On the other hand, if the CF splittings are not large compared to the hybridization scale parameters Γ for the low CF levels, then the CF and hybridization structures should become difficult to disentangle, even with detailed inelastic neutron probing. This is well known experimentally; the point here is that there is now a systematic way to treat this theoretically. A related consequence is that the ground state may also contain a significant admixture of CF eigenstates.

There are also some cases where the CF ground state may be a Γ_8 quartet This is now clear for $CeBe_6$, and may well also be the case for UBe_{13}, based on general considerations [26] and the available evidence (assuming A_4, A_6 similar to those for $PrBe_{13}$ [28]). This case can be modeled simply by having the lowest two f levels of the preceeding ($CeAl_3$-type) case be degenerate.

In all three of the "normal" heavy-fermion materials, the resistivity peak is found considerably above the second peak in specific heat. In UBe_{13}, however, the order of these peaks is reversed [18]. We speculate that this difference may be the result of having a Γ_8 ground state.

In conclusion, the way now seems clear for more detailed and realistic modeling of low-temperature properties of VF materials. If ways can be found to adequately represent Baber scattering and the Kondo crossover, the result might provide a fairly complete theory of electronic properties.

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